Schottky Barrier Notes

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1 Parameters

Carrier mobility (μ)		300 cm^2/Vs
Dark resistivity (ρ)		10000 Ω.cm
Dopant concentration (N_d)	$\frac{1}{\rho e \mu}$	2.08e12 cm^{-3}
Debye length (L_D)	$\sqrt{\frac{\epsilon k_B T}{e^2 N_d}}$	2.8 μm
Pump FWHM duration (T_s)		190 fs
Plasma scattering time (τ_s)		100 fs
Group index at 1030nm (n_g)		3.874
Schottky barrier electric field (E_{SB})	fit	$\sim 10^4$ V/m
Effective mass ($m^\star$)		0.26 m_0

2 Equations of motion

In FDTD, we solve Maxwell's equations in 2D with a source $J(\vec{r}, t)$

$$\epsilon \frac{\partial \vec{E}}{\partial t} = \nabla \times \vec{H} - \vec{J} \tag{1}$$

$$\frac{\partial \vec{H}}{\partial t} = -\nabla \times \vec{E} \tag{2}$$

The current density due to photoionized charge carriers is given by

$$\vec{J} = e \sum_i \Delta n_i \vec{v_i} \tag{3}$$

where e is the electron charge, Δn_i is the differential electron density produced at instant i from photoionization of the silicon by the NIR pump pulse and $\vec{v_i}$ is the instantaneous velocity of those electrons in the medium. The equation of motion for $\vec{v_i}$ is

$$\frac{d\vec{v_i}}{dt} = -\frac{\vec{v_i}}{\tau} + \frac{e\vec{E}}{m^\star} \tag{4}$$

where τ is the momentum scattering time, e is the electronic charge (negative in this notation) and $m^\star$ is the effective electron mass in silicon. The solution to this differential equation is

$$\vec{v}_i(r,t) = \int_{t_i}^{t} dt'\, e^{-(t-t')/\tau} \frac{e\vec{E}(r,t')}{m^\star} \tag{5}$$

We substitute that expression back into the equation for $\vec{J}$ and use that

$$\Delta n_i = \left(\frac{\partial n}{\partial t}\right)_{t_i} \Delta t. \tag{6}$$

Then,

$$\vec{J} = \frac{e^2}{m^\star} \sum_i \left(\frac{\partial n}{\partial t}\right)_{t_i} \Delta t \int_{t_i}^{t} dt'\, e^{-(t-t')/\tau} \vec{E}(r,t') \tag{7}$$

and we take the limit as $\Delta t \to 0$ to get

$$\vec{J} = \frac{e^2}{m^\star} \int_0^t dt' \left(\frac{\partial n}{\partial t}\right)_{t'} \int_{t'}^{t} dt''\, e^{-(t-t'')/\tau} \vec{E}(r,t'') \tag{8}$$

Taking a time derivative of the current and using the Leibniz rule gives

$$\frac{\partial \vec{J}}{\partial t} = -\frac{\vec{J}}{\tau} + \frac{e^2 n(r,t)}{m^\star} E(r,t). \tag{9}$$

The electric field in Eq. (9) is the sum of the static Schottky Barrier electric field (E_{SB}) and that obtained from solving Ampere's law in Eq. (1), i.e. $\vec{E}_{tot} = \vec{E}_{SB} + \vec{E}$.

3 Plasma generation

The photoionized charge carriers obey the equation of motion

$$\frac{\partial n_f}{\partial t} = G(\vec{r},t) \tag{10}$$

where $G(\vec{r},t)$ is a generating function originating from the NIR pump pulse. It is Gaussian in space and time such that integration of this equation gives

$$n_f(\vec{r},t) = n_0 P(z) B(f(\vec{r},t)) \tag{11}$$

where

$$B(x) = \frac{1}{2}\left(1 + \mathrm{Erf}\left(\frac{x}{\sqrt{2}\sigma}\right)\right) \tag{12}$$

n_0 is the number density of charge carriers, $P(z)$ is the normalized intensity profile of the NIR pump along the propagation direction of the THz signal and $f(\vec{r},t)$ describes the wave front of the NIR pump in the silicon. The value for

σ^2 is given by the pulse FWHM time T_s such that $\sigma^2 = T_s^2/(8\log(2))$. The corresponding plasma frequency is

$$\omega_{p0} = \sqrt{\frac{e^2 n_0}{\epsilon_0 m^\star}}. \tag{13}$$

In terms of the plasma frequency, Eq. (9) becomes

$$\frac{\partial \vec{J}}{\partial t} = -\frac{\vec{J}}{\tau} + \epsilon_0 \omega_{p0}^2 P(z) B(f(\vec{r},t)) \left(\vec{E} + \vec{E}_{SB}\right). \tag{14}$$

3.1 Normal Incidence ($v \to \infty$)

$$f(\vec{r},t) = t - t_0 - \frac{d-y}{v_g} \tag{15}$$

where $v_g = c/n_g$ is the group velocity of the NIR pump inside silicon.

3.2 Tilted Incidence (finite v)

$$f(\vec{r},t) = t - t_0 - \frac{d-y}{v_g} - \frac{z-z_0}{v} \tag{16}$$

where v is the mirror velocity which is uniquely defined by the angle of incidence and z_0 is the position at which the pump front enters the waveguide at position $y = d$ and at time t_0.

4 Solving in FDTD

We solve the above equations in FDTD as follows

1 Initialize all fields and currents to zero.

2 Compute the electric fields (ignoring spacial indices for clarity)

$$(E_y)^n = (E_y)^{n-1} + \frac{\Delta t}{\epsilon}\left(\frac{\partial H_x}{\partial z}\right)^{n-1/2} - \frac{1}{\epsilon}(J_y)^{n-1/2} \tag{17}$$

$$(E_z)^n = (E_z)^{n-1} - \frac{\Delta t}{\epsilon}\left(\frac{\partial H_x}{\partial y}\right)^{n-1/2} - \frac{1}{\epsilon}(J_z)^{n-1/2} \tag{18}$$

3 Compute the magnetic field

$$(H_x)^{n+1/2} = (H_x)^{n-1/2} + \Delta t\left(\left(\frac{\partial E_y}{\partial z}\right)^n - \left(\frac{\partial E_z}{\partial y}\right)^n\right) \tag{19}$$

4 Compute the currents J_y and J_z

$$(J_y)^{n+1/2} = \frac{1/\Delta t - \gamma/2}{1/\Delta t + \gamma/2}(J_y)^{n-1/2} + \frac{1}{1/\Delta t + \gamma/2}\omega_{p0}^2 P(z) B^n \left((E_y)^n + E_{SB}\right) \tag{20}$$

$$(J_z)^{n+1/2} = \frac{1/\Delta t - \gamma/2}{1/\Delta t + \gamma/2}(J_z)^{n-1/2} + \frac{1}{1/\Delta t + \gamma/2}\omega_{p0}^2 P(z) B^n (E_z)^n \tag{21}$$

where care was taken to preserve the second order accuracy of FDTD, hence the funny looking prefactors. The Schottky Barrier electric field is finite only in the y-direction and $\gamma = 1/\tau$.

6 Loop over 2-5.